Supporting Information

EDTA-Inspired Polydentate Hydrogels with Exceptionally High Heavy Metal Adsorption Capacity as Reusable Adsorbents for Wastewater Purification

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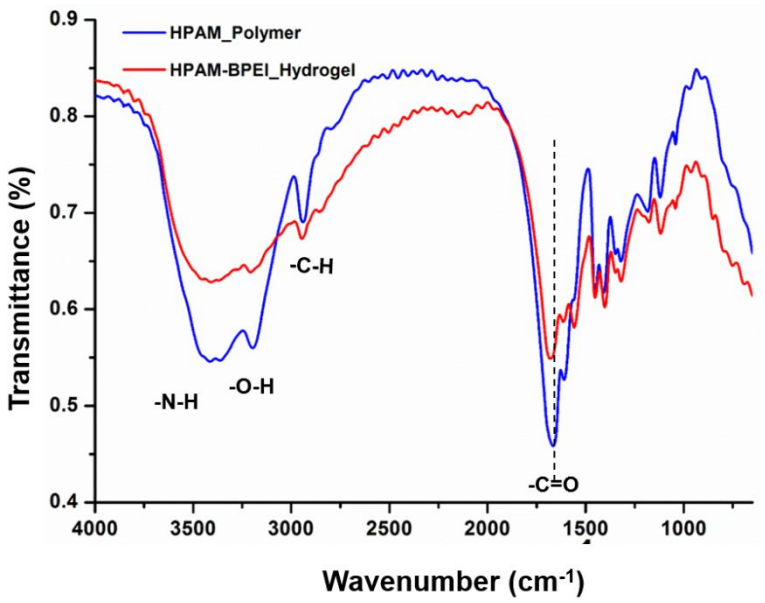

Figure S1. FTIR spectra of the HPAM polymer and synthesized hydrogel (Sample HG-1)

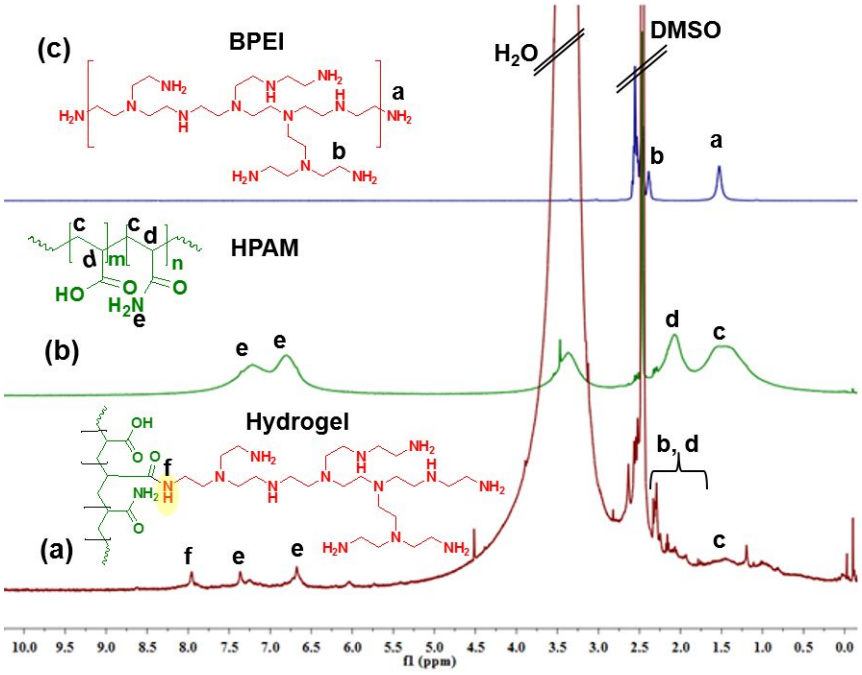

Figure S2. ^{1}H NMR of the (a) BPEI, (b) HPAM polymer and (c) synthesized hydrogel in DMSO-d_6

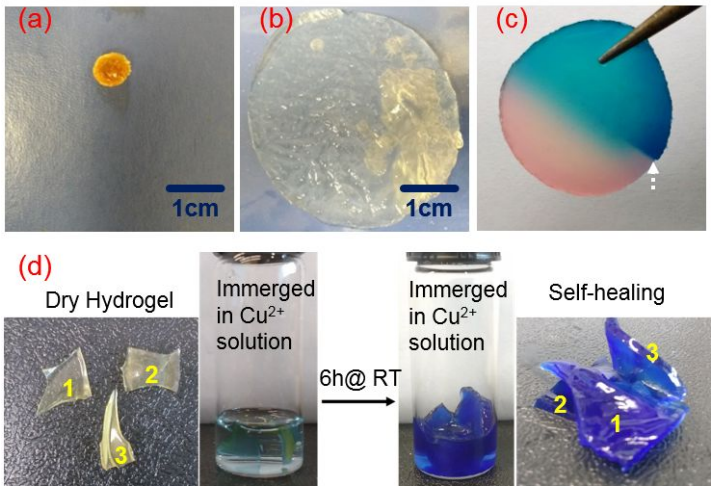

Figure S3. Images of (a) dry and (b) swollen hydrogel (Sample HG-1). (c) Self-healing of the two separate hydrogel pieces (stained with red and blue dyes) into a single gel. The white arrow indicates the part where a razor blade was placed to prevent contact between two hydrogel piece, resulting in no healing. (d) Self-healing of three pieces of hydrogel immersed in Cu^{2+} solution after 6 h at room temperature.

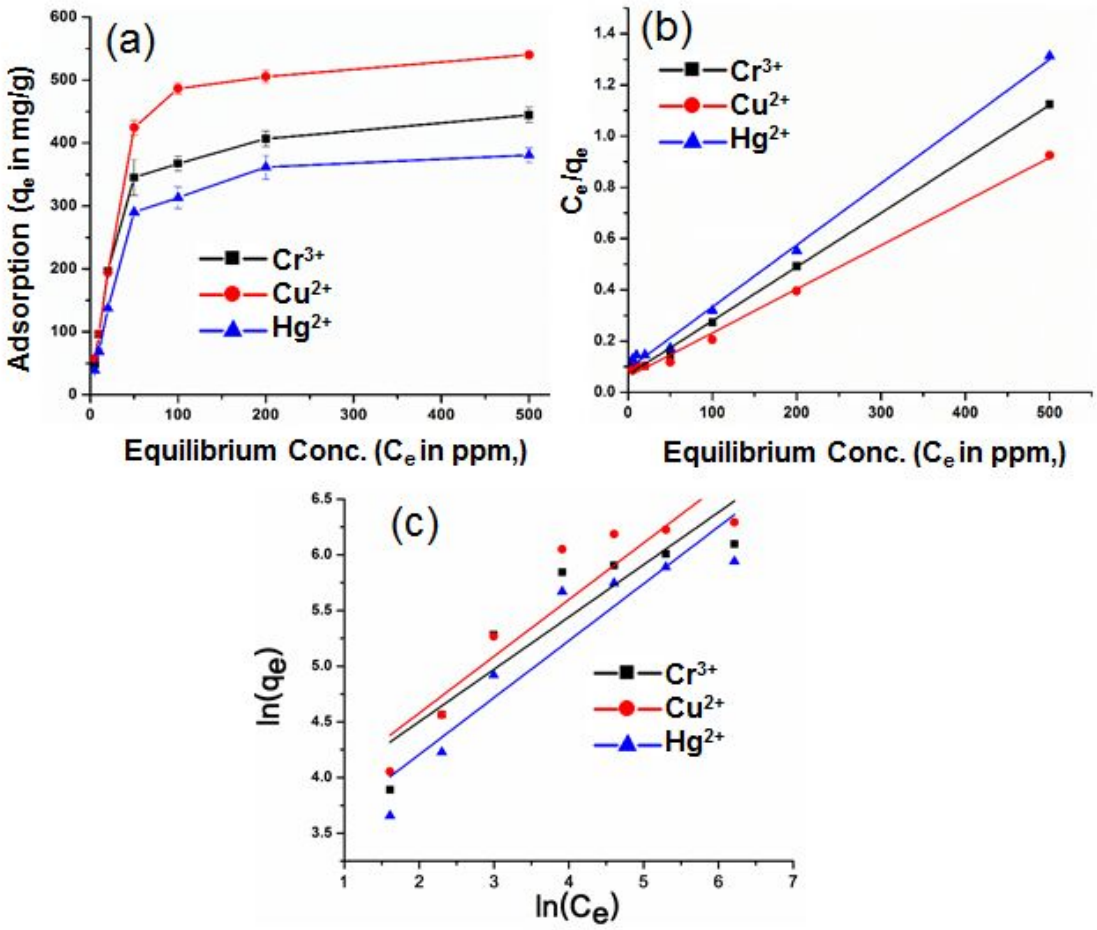

Figure S4. (a) Adsorption isotherms: metal ion adsorption capacity at equilibrium (q_e) as a function of equilibrium concentration (C_e) of the metal ions in solution. (b) C_e/q_e as a function of C_e and the linear fit with the Langmuir adsorption model. (c) ln(q_e) as a function of ln(c_e) and the linear fit with the Freundlich adsorption model.

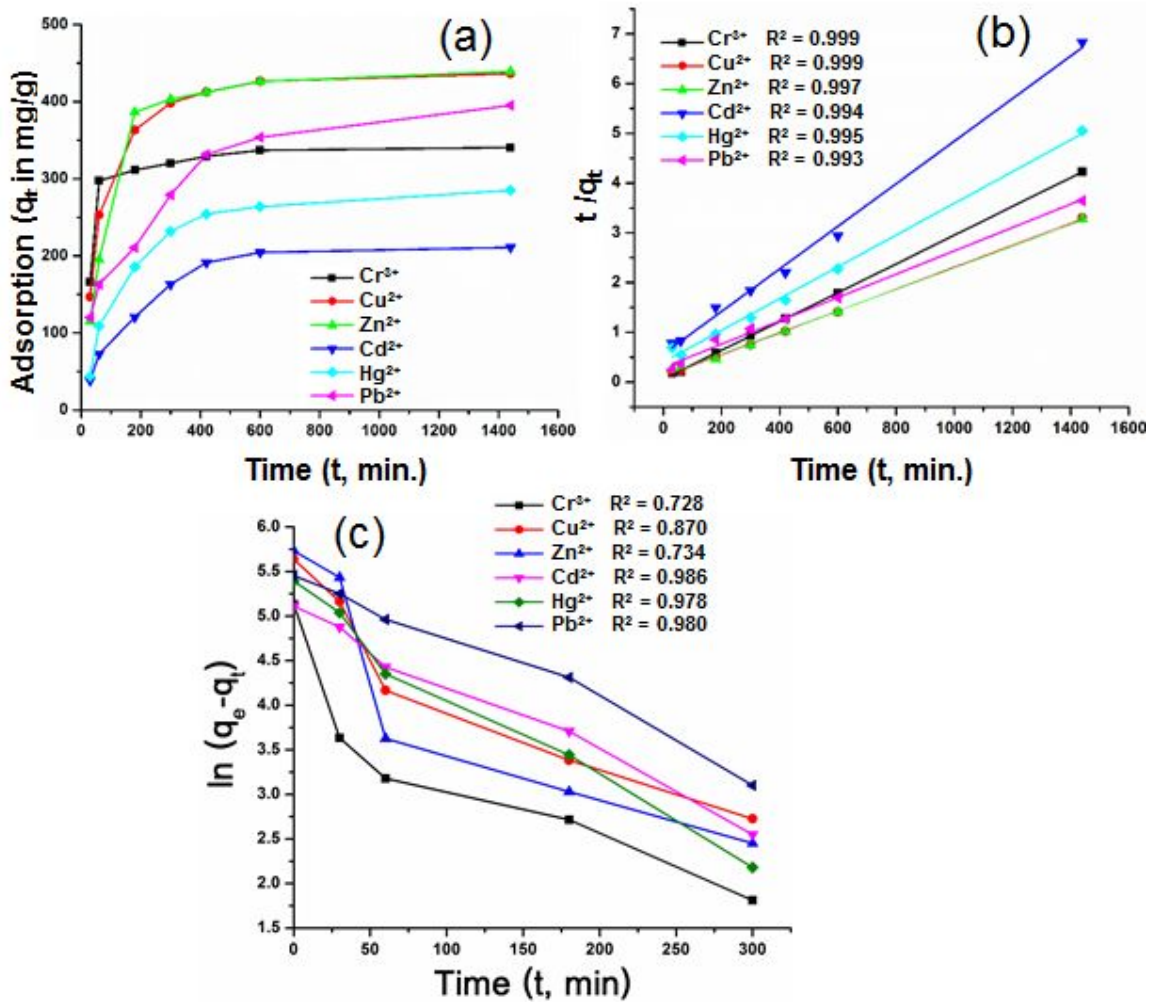

Figure S5. (a) Adsorption kinetics: the adsorption capacity of the metal ions (q_t) as a function of time. (b) t/q_t as a function of time (t) and the linear fit with pseudo second-order kinetics model. (c) $\ln(q_e-q_t)$ as a function of time (t) and the linear fit with pseudo first-order kinetics model.

Table S1. Calculated parameters corresponding to the Langmuir adsorption isotherm

Metal Ions	**Langmuir adsorption isotherm**			**Freundlich adsorption isotherm**		
	q_{max} (mg g^{-1})	K_L (L mg^{-1})	R^2	K_F	1/n	R^2
Cr^{3+}	473.93	0.030	0.997	3.56	0.47	0.813
Cu^{2+}	584.79	0.0281	0.994	3.55	0.50	0.833
Hg^{2+}	413.22	0.0264	0.995	3.18	0.51	0.844

Table S2. Pseudo-first order and pseudo-second order kinetic parameters of adsorption of heavy metal ions by hydrogel

Metal Ions	Pseudo-first order kinetic		Pseudo-second order kinetic		
	K_1 (min^{-1})	R^2	q_{cal} ($mg\ g^{-1}$)	K_2 ($g\ mg^{-1}\ min^{-1}$)	R^2
Cr^{3+}	0.0088	0.728	357.14	1.29×10^{-4}	0.999
Cu^{2+}	0.0092	0.870	454.54	4.69×10^{-5}	0.999
Zn^{2+}	0.0105	0.734	476.19	3.36×10^{-5}	0.997
Cd^{2+}	0.0083	0.986	238.09	3.13×10^{-5}	0.994
Hg^{2+}	0.0103	0.978	322.58	2.39×10^{-5}	0.995
Pb^{2+}	0.0076	0.980	434.78	1.80×10^{-5}	0.993

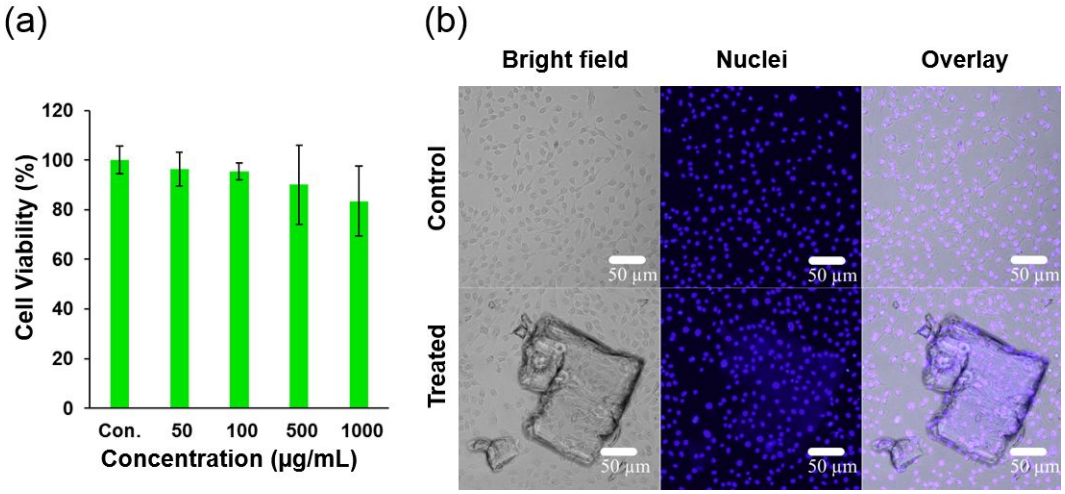

Figure S6. Cytotoxicity of the EDTA-inspired polydentate hydrogels toward mouse fibroblasts. (a) Dose-dependent cell viability. (b) Images of cells captured after 24 h of incubation with the hydrogel. The nuclei of the cells were stained with NucBlue® Live ReadyProbes® Reagent.